

# Conservation laws in disordered electron systems: Thermodynamic limit and configurational averaging

V. Janiš and J. Koloreň

*Institute of Physics, Academy of Sciences of the Czech Republic,  
Na Slovance 2, CZ-18221 Praha 8, Czech Republic\**

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We discuss conservation of probability in noninteracting disordered electron systems. We argue that although the norm of the electron wave function is conserved in individual realizations of the random potential, we cannot extend this conservation law easily to configurationally averaged systems in the thermodynamic limit. A direct generalization of the norm conservation to averaged functions is hindered by the existence of localized states breaking translational invariance. Such states are elusive to the description with periodic Bloch waves. Mathematically this difficulty is manifested through the diffusion pole in the electron-hole irreducible vertex. The pole leads to a clash with analyticity of the self-energy, reflecting causality of the theory, when norm conservation is enforced by the Ward identity between one- and two-particle averaged Green functions.

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## I. INTRODUCTION

Itinerant quantum disordered systems are very difficult to describe quantitatively. One has to be aware of a few pitfalls that may destroy the standard scheme adopted from clean solids. Quantum systems must be represented in a Hilbert space. When a static, quenched disorder is present, each single configuration of the random potential (force) has its own state space. First assumption we standardly make is that a suitable representation space exists comprising states of all configurations of the random potential. The disordered system then formally behaves as a clean one with renormalized products of operators via vertex corrections.

Operators are generally difficult to treat unless we are able to use their spectral representations. In the thermodynamic limit, i. e. in infinite volume, the eigenstates of itinerant Hamiltonians may either be localized, quadratic integrable, or extended with a plane-wave character. The former eigenfunctions belong to the point spectrum with separate eigenvalues, while the latter ones to a continuous band of eigenenergies. These two types of eigenfunctions are well separable for one inhomogeneous configuration. Configurational averaging, however, can turn the point spectrum effectively continuous and it becomes extremely difficult to distinguish the character of spectral energies, that is the extension of the eigenfunctions, solely from averaged quantities. Determination of the extension of typical eigenstates of a random itinerant Hamiltonian is the core of the so-called Anderson localization problem.<sup>1</sup>

Since exact solutions of the Anderson localization problem are not available one has to resort approximate treatments. There are two complementary tools, numerical and analytic, to tackle this problem. Neither of them is, however, able to answer all questions about the spectrum of random itinerant Hamiltonians. While the former technique can deal only with finite lattices and many configurations of the random potential,<sup>2</sup> the latter one deals mostly with the thermodynamic limit and config-

urationally averaged quantities.<sup>3</sup> In particular the latter approach demands a special caution in building a consistent picture of the metal-insulator transition at which configurations with extended states become irrelevant.

In order not to miss the physics of the problem one has to minimize spurious effects, introduced in approximate treatments, by taking into account as many exactly valid relations as possible. Conservation laws are typical properties to be maximally satisfied also in approximate theories. They impose the so-called “no-go” theorems that may essentially restrict the state space of the system and hint to available “order parameter”. The aim of this paper is to elucidate the role and applicability of conservation of probability, or conservation of the norm of the wave function, in the Anderson localization problem. Although it may seem evident that the norm of the wave function must be unconditionally conserved, it is the random character of the Anderson model that makes the proper utilization of probability conservation a rather subtle issue deserving a deeper and more thorough investigation.

We use the simplest possible model on which we can demonstrate subtleties of the application of conservation laws in random systems. It is the Anderson model of noninteracting lattice electrons subject to a random potential, the Hamiltonian of which can be written as

$$\hat{H}_{AD} = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + \sum_i V_i c_i^\dagger c_i. \quad (1)$$

We assume that the kinetic energy (nearest-neighbor hopping term)  $t_{ij} = t_{|i-j|}$  is homogeneous and only the local potential  $V_i$  is random. The values of the random potential  $V_i$  are site-independent and obey a disorder distribution  $\rho(V)$ . A function depending on the random potential  $V_i$  is then averaged via

$$\langle X(V_i) \rangle_{av} = \int_{-\infty}^{\infty} dV \rho(V) X(V). \quad (2)$$

Anderson showed in his seminal paper, Ref. 1, that the eigenstates of single configurations can either be extended or localized. In the former case we have a metallic conductivity (diffusive regime). The latter case, called Anderson localization, leads to an insulator and we have a diffusionless transport regime. A consistent theory of the disorder induced vanishing of diffusion is still missing. One of the reasons for this shortage is incomplete understanding of probability conservation in this simple model. We discuss in the following sections what holds for sure and what applications of conservation laws demand special additional assumptions.

## II. NORM CONSERVATION AND WARD IDENTITY: ONE CONFIGURATION

We start with a finite system and consider one fixed configuration of the random potential. It is a very straightforward situation where no problems with conservation of the norm of the wave function are to be expected. Since the Anderson model, Eq. (1), consists of noninteracting electrons, we can formally find an exact solution via an evolution operator. We define

$$\hat{U}(t) = e^{-i\hat{H}t} . \quad (3)$$

The evolution operator  $\hat{U}(t)$  represents a *formal* solution unless we are able to diagonalize the Anderson Hamiltonian. It is, however, possible only numerically and for rather small lattices. We can nevertheless use this formal solution to see how conservation of the norm of the wave function can be represented. We evaluate the following integral for arbitrary complex energies  $z$  with  $\Im z > 0$

$$\begin{aligned} \int_0^\infty dt e^{izt} \langle \psi(t) | \psi(t) \rangle &= \int_0^\infty dt e^{izt} \langle \psi | \hat{U}(t) \hat{U}^\dagger(t) | \psi \rangle \\ &= \int_0^\infty dt \sum_{ijn} \psi_i \psi_j^* e^{izt} \langle j | \hat{U}(t) | n \rangle \langle n | \hat{U}^\dagger(t) | i \rangle \\ &= -\frac{1}{iz} \sum_n |\psi_n|^2 \end{aligned} \quad (4)$$

where  $|i\rangle$  denotes the localized orbital on the site  $\mathbf{R}_i$  and  $\langle i | j \rangle = \delta_{ij}$ .

Identity (4) is a rather evident consequence of conservation of the norm of the wave function. It is less evident and more interesting when we rewrite this identity with resolvent operators and Green functions. We introduce the resolvent as a Fourier transform of the evolution operator

$$\hat{G}(z) = -i \int_{-\infty}^{\infty} dt \theta(t) e^{izt} \hat{U}(t) = [z\hat{1} - \hat{t} - \hat{V}]^{-1} . \quad (5)$$

Using the local orbitals (Wannier states) we define one-

and two-particle Green functions

$$G_{ij}(z) = \langle i | \hat{G}(z) | j \rangle , \quad (6a)$$

$$G_{ij,kl}^{(2)}(z_1, z_2) = \langle i | \hat{G}(z_1) | j \rangle \langle k | \hat{G}(z_2) | l \rangle . \quad (6b)$$

The two-particle Green function is trivially only a product of one-electron Green functions, since we do not have interacting electrons and we stay within one fixed configuration of the random potential.

It is easy to insert the resolvent operators (finite matrices) into Eq. (4) to obtain

$$\begin{aligned} \sum_n G_{in,nj}^{(2)}(z_1, z_2) &= \sum_n G_{in}(z_1) G_{nj}(z_2) \\ &= \frac{1}{z_2 - z_1} [G_{ij}(z_1) - G_{ij}(z_2)] . \end{aligned} \quad (7)$$

The result is kind of Ward identity being a direct consequence of probability conservation for quantum noninteracting systems. It holds for any configuration of the random potential.

In finite systems all eigenenergies of the Anderson Hamiltonian are discrete and nondegenerate. The situation changes if we perform the thermodynamic limit, where the volume of the lattice increases to infinity, i. e., we have infinite-many lattice sites. To perform the thermodynamic limit we choose the values of the random potential on the newly added sites according to the disorder distribution  $\rho$  from Eq. (2). To extend the validity of the Ward identity (7) to infinite systems we have to demand completeness of the set of Wannier states. That is, we require

$$\sum_n |n\rangle \langle n| = \hat{1} , \quad \|\psi\|^2 \equiv \sum_n \langle \psi | n \rangle \langle n | \psi \rangle = 1 . \quad (8)$$

The latter equality says that we close finite sums over the Wannier states in such a way that the norm can be fixed. The Wannier states form an orthonormal basis in the Hilbert space of random configurations, i. e.  $\langle i | j \rangle = \delta_{ij}$ . Condition (8) guarantees validity of the Ward identity (2) strictly only for proper states from the Hilbert space (localized states). In this case the infinite sum on the l.h.s. of Eq. (7) converges strongly in the Hilbert space spanned over the Wannier states. We, however, know that the thermodynamic limit generally generates extended states belonging to the continuous spectrum of the Anderson Hamiltonian. These extended states are not proper vectors in the Hilbert space. To prove the Ward identity also for extended states of a single configuration we have to weaken the convergence criterion for the sum over the intermediate states. It is in principle possible to formalize such a procedure.

## III. CONFIGURATIONALLY AVERAGED QUANTITIES

Analysis of individual configurations of the random potential is manageable only by numerical means, since

random configurations are not generally translationally invariant. Hence, an analytic treatment is not viable due to the lack of apparent symmetry that would help reduce the number of degrees of freedom.

The configurational averaging provides a means for reducing the complexity of the description of random systems, as it restores translational invariance. Translationally invariant lattice electrons can be formally described by standard field-theoretic methods used for pure (interacting) systems. If the ergodic (self-averaging) hypothesis holds, i. e., if extensive thermodynamic quantities evaluated for one typical configuration equal their averaged values, averaging does not change the physics of the problem. It does not, however, mean that all relations and identities valid for single configurations can automatically be transferred to averaged quantities.

To generalize the Ward identity (7) to averaged quantities we have to assume that the sum over the intermediate states commutes with the configurational averaging, that is

$$\frac{1}{\mathcal{N}_c} \sum_{\{C\}} \sum_n \Psi_n(\{C\}) = \sum_n \frac{1}{\mathcal{N}_c} \sum_{\{C\}} \Psi_n(\{C\}), \quad (9)$$

where  $\Psi_n(\{C\})$  are configurationally dependent functions of interest, the matrix elements of the two-particle Green function in this case. This equality may seem evident and indeed holds for every finite-volume samples as all involved sums run over finite number of elements. In the thermodynamic limit both sums, over the basis states  $\sum_n$  and over the random configurations  $\mathcal{N}_c^{-1} \sum_{\{C\}}$ , are infinite and they are interchangeable only if states of all relevant random configurations fall into a single Hilbert space. That is, if the basis vectors  $|n\rangle$  are configurationally independent. We will show later on that this need not be always the case.

After averaging the system does not behave as a simple Fermi gas, since the product of averages does not equal the average of the product. Hence, the two-electron resolvent, Eq. (6b), will be defined via a Bethe-Salpeter equation,

$$\begin{aligned} \langle G_{ij,kl}^{(2)}(z_1, z_2) \rangle_{av} &= \langle G_{ij}(z_1) \rangle_{av} \langle G_{kl}(z_2) \rangle_{av} \\ &+ \sum_{i'j'k'l'} \langle G_{ii'}(z_1) \rangle_{av} \langle G_{l'l}(z_2) \rangle_{av} \\ &\times \Lambda_{i'j',k'l'}(z_1, z_2) \langle G_{j'j,kk'}^{(2)}(z_1, z_2) \rangle_{av}. \end{aligned} \quad (10)$$

We introduced a two-particle irreducible vertex  $\Lambda$  to take into account correlations between the one-electron Green functions from the product in Eq. (6b) due to the averaging. Analogously, the averaged one-electron resolvent (5) is determined from a self-energy  $\hat{\Sigma}$  via the Dyson equation,  $\langle \hat{G}(z) \rangle_{av} = [z\hat{1} - \hat{t} - \hat{\Sigma}]^{-1}$ . Both, the self-energy  $\Sigma$  and the irreducible vertex  $\Lambda$ , display translational invariance.

Assuming validity of Eq. (9) and using the Bethe-Salpeter equation (10) we transform the Ward identity

(7) to an identity between the self-energy and the two-particle irreducible vertex,<sup>4</sup>

$$\begin{aligned} \Sigma_{il}(z_1) - \Sigma_{il}(z_2) \\ = \sum_{j'k'} \Lambda_{ij',k'l}(z_1, z_2) [\langle G_{j'k'}(z_1) \rangle_{av} - \langle G_{j'k'}(z_2) \rangle_{av}]. \end{aligned} \quad (11)$$

It is a special case of the so-called Vollhardt-Wölfle Ward identity proved from a diagrammatic perturbation expansion for the two-particle vertex  $\Lambda$ .<sup>5</sup>

To exploit fully the simplifications brought in by the configurational averaging we have to switch to a basis set consisting of Bloch waves. It is a natural basis for translationally invariant lattice systems. The Bloch waves can be introduced through the Wannier states as follows

$$\langle \mathbf{k}|n\rangle = e^{-i\mathbf{k}\cdot\mathbf{R}_n}, \quad (12)$$

where  $\mathbf{k}$  is quasiparticle momentum labelling the Bloch waves. As far as we stay in finite volumes, the completeness of the basis and the norm of any state vector read

$$\frac{1}{N} \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}| = \hat{1}, \quad \|\psi\|^2 \equiv \frac{1}{N} \sum_{\mathbf{k}} \langle \psi|\mathbf{k}\rangle \langle \mathbf{k}|\psi\rangle \quad (13)$$

with  $N$  being the number of sites in the given volume. The only difference compared to relations (8) is the normalization factor of the basis vectors,  $\langle \mathbf{k}|\mathbf{k}'\rangle = N\delta_{\mathbf{k},\mathbf{k}'}$ . It says that the Bloch waves are normalized to the volume, i. e., their norm increases linearly with the volume. This normalization is chosen so that the thermodynamic limit is well defined. There the completeness relation comes over to a spectral integral

$$\frac{1}{N} \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}| \xrightarrow{N \rightarrow \infty} \frac{1}{(2\pi)^d} \int d^d k |\mathbf{k}\rangle \langle \mathbf{k}| = \hat{1} \quad (14)$$

with generalized orthonormality  $\langle \mathbf{k}|\mathbf{k}'\rangle = \delta(\mathbf{k}-\mathbf{k}')$ , where  $\delta$  is the Dirac delta function.

In the Bloch-wave representation the one-particle Green function is diagonal

$$\begin{aligned} G(\mathbf{k}, z) &= \frac{1}{z - \epsilon(\mathbf{k}) - \Sigma(\mathbf{k}, z)} \\ &= \frac{1}{N} \sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \langle G_{ij}(z) \rangle_{av} \end{aligned} \quad (15)$$

and the two-particle Green function depends on only three momenta as the total momentum is conserved. The notation for the momentum-dependent averaged two-particle Green function we use throughout the rest of the paper reads

$$\begin{aligned} G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{q}) &= \frac{1}{N^2} \sum_{ijkl} e^{-i(\mathbf{k}+\mathbf{q})\cdot\mathbf{R}_i} e^{i(\mathbf{k}'+\mathbf{q})\cdot\mathbf{R}_j} \\ &\times e^{-i\mathbf{k}'\cdot\mathbf{R}_k} e^{i\mathbf{k}\cdot\mathbf{R}_l} \langle G_{ij,kl}^{(2)}(z_1, z_2) \rangle. \end{aligned} \quad (16)$$

The Ward identity (7) for the averaged Green functions in momentum representation is

$$\frac{1}{N} \sum_{\mathbf{k}'} G_{\mathbf{k}, \mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{0}) = -\frac{1}{\Delta z} [G(\mathbf{k}, z_1) - G(\mathbf{k}, z_2)] \quad (17)$$

where  $\Delta z = z_1 - z_2$ .

Notice that in finite volumes one cannot straightforwardly distinguish between diffusive electron states, describing a particle “smeared” throughout the whole sample, and localized states with exponential tails confined to a finite subvolume. Such a distinction is meaningful only in the thermodynamic limit. There the diffusive states have a character of Bloch waves, i.e., they describe particle *fluxes*. On the other hand the localized states contain just a single particle localized in a finite volume. Intuitively, technical difficulties can arise if a physical process involves both types of eigenstates, localized and extended. It is the case of the Anderson localization transition where extended states go over to localized ones.

#### IV. DIFFUSION POLE AND CAUSALITY

Since the averaged two-particle resolvent is not a simple product as for single configurations, Eq. (5), but rather fulfills the Bethe-Salpeter equation (10), it is not so apparent how the Ward identity (17) is related with particle conservation. It can be demonstrated at best via diffusion. In the weak disorder limit the motion of electrons in a random medium is expected to be diffusive, i.e., the Fourier components of non-equilibrium particle-density variations die out according to the exponential law

$$\delta n(t, \mathbf{q}) = \delta n(0, \mathbf{q}) e^{-Dq^2 t}, \quad t > 0. \quad (18)$$

In order to reproduce such a diffusive behavior the electron-hole correlation function  $\Phi_{EF}^{AR}(\mathbf{q}, \omega) = N^{-2} \sum_{\mathbf{k}, \mathbf{k}'} G_{\mathbf{k}, \mathbf{k}'}^{(2)}(E_F + \omega + i0^+, E_F - i0^+; \mathbf{q})$  has to display the so-called diffusion pole,<sup>6</sup>

$$\Phi_{EF}^{AR}(\mathbf{q}, \omega) \approx \frac{2\pi n_F}{-i\omega + Dq^2}. \quad (19)$$

Here  $D$  stands for the diffusion constant and  $n_F$  is the electron density of states at the Fermi energy  $E_F$ . The diffusion pole exists only if the Ward identity (17) is fulfilled by the averaged one- and two-particle Green functions.<sup>6</sup>

Unfortunately, the correlation function  $\Phi$  does not obey an equation of motion, so it is difficult to use this realization of the diffusion pole to control conservation laws in approximate theories. It can, however, be shown that the same pole must appear in the two-particle irreducible function  $\Lambda$ . To demonstrate that we analyze the two-particle functions in more details. It is convenient to introduce a vertex  $\Gamma$  that is just the two-particle Green

function  $G^{(2)}$  with uncorrelated part subtracted,

$$G_{\mathbf{k}, \mathbf{k}'}^{(2)}(z_+, z_-; \mathbf{q}) = G(\mathbf{k}, z_+) G(\mathbf{k} + \mathbf{q}, z_-) [\delta(\mathbf{k} - \mathbf{k}') + \Gamma_{\mathbf{k}, \mathbf{k}'}(z_+, z_-; \mathbf{q}) G(\mathbf{k}', z_+) G(\mathbf{k}' + \mathbf{q}, z_-)]. \quad (20)$$

In analogy to the averaged two-particle resolvent, the two-particle vertex obeys a Bethe-Salpeter equation. Once we go beyond local approximations, an example of which is the mean-field coherent-potential approximation (CPA), there are three Bethe-Salpeter equations for the vertex  $\Gamma$  we can construct. The three Bethe-Salpeter equations are related to three different ways how to define a two-particle irreducibility. Equivalently they correspond to three topologically distinct two-particle processes, the electron-hole and the electron-electron (hole-hole) scatterings and the one-electron self-corrections.<sup>4</sup>

Since only the off-diagonal one-electron propagators  $\bar{G}(\mathbf{k}, z) \equiv G(\mathbf{k}, z) - N^{-1} \sum_{\mathbf{k}} G(\mathbf{k}, z)$  are relevant for distinguishing various representations of the full vertex we use Bethe-Salpeter equations with just these propagators. The most important Bethe-Salpeter equation is that from the electron-hole scattering channel that reads

$$\Gamma_{\mathbf{k}, \mathbf{k}'}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}, \mathbf{k}'}^{eh}(\mathbf{q}) + \frac{1}{N} \sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}, \mathbf{k}''}^{eh}(\mathbf{q}) \times \bar{G}_+(\mathbf{k}'') \bar{G}_-(\mathbf{k}'' + \mathbf{q}) \Gamma_{\mathbf{k}'', \mathbf{k}'}(\mathbf{q}). \quad (21a)$$

We added the superscript *eh* to the irreducible vertex  $\Lambda$  in order to distinguish it from the other two irreducible channels. Notice that the full vertex  $\Gamma$  must remain channel independent. For the sake of simplicity we suppressed energy variables. The subscript  $\pm$  at the one-electron propagators refers to the first and second energy variable in the corresponding two-particle vertex, respectively.

Besides the electron-hole channel, Eq. (21a), it is for our purposes sufficient to use only one out of the two remaining Bethe-Salpeter equations — the electron-electron (hole-hole) channel,

$$\Gamma_{\mathbf{k}, \mathbf{k}'}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}, \mathbf{k}'}^{ee}(\mathbf{q}) + \frac{1}{N} \sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}, \mathbf{k}''}^{ee}(\mathbf{q} + \mathbf{k}' - \mathbf{k}'') \times \bar{G}_+(\mathbf{k}'') \bar{G}_-(\mathbf{Q} - \mathbf{k}'') \Gamma_{\mathbf{k}'', \mathbf{k}'}(\mathbf{q} + \mathbf{k} - \mathbf{k}''), \quad (21b)$$

where  $\mathbf{Q} = \mathbf{k} + \mathbf{k}' + \mathbf{q}$ .

The two-particle irreducible vertices play the role of the two-particle self-energy and are to be determined from e. g. a diagrammatic expansion. The best way to access them is to use the so-called parquet approach.<sup>4</sup> In it we introduce a completely irreducible (irreducible in all distinct channels) two-particle vertex  $\mathcal{I}$  and use topological nonequivalence of different scattering channels. When we distinguish only the electron-hole and electron-electron channels we can write the parquet equation as<sup>4</sup>

$$\Gamma_{\mathbf{k}, \mathbf{k}'}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}, \mathbf{k}'}^{eh}(\mathbf{q}) + \bar{\Lambda}_{\mathbf{k}, \mathbf{k}'}^{ee}(\mathbf{q}) - \mathcal{I}_{\mathbf{k}, \mathbf{k}'}(\mathbf{q}). \quad (22)$$

The minus sign at the completely irreducible vertex  $\mathcal{I}$  compensates for the same contributions in the electron-hole and the electron-electron irreducible vertices. Notice that all local two-particle contributions belong to the completely irreducible vertex  $\mathcal{I}$ .

If the physical system under investigation is invariant with respect to time reversal (no magnetic field), the two-particle vertices obey the electron-hole symmetry expressed in a relation  $\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Gamma_{\mathbf{k}\mathbf{k}'}(-\mathbf{q} - \mathbf{k} - \mathbf{k}')$  for the full vertex and in  $\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{ee}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{eh}(-\mathbf{q} - \mathbf{k} - \mathbf{k}')$  for the irreducible ones. As a consequence of the parquet equation (22) the diffusion pole from the full vertex  $\Gamma$  must appear at least in one of the irreducible functions  $\Lambda$ . However, due to the electron-hole symmetry, both vertices  $\Lambda^{eh}$  and  $\Lambda^{ee}$  display the same analytic behavior and hence must contain the same singularity, the diffusion pole. As discussed above, the existence of the diffusion pole in the two-particle irreducible vertices is a consequence of conservation laws applied to averaged systems via the Ward identity. Since the vertex functions obey equations of motion, the existence of the diffusion pole in them can be used to check conserving character of approximate treatments.

Having a pole in the electron-hole irreducible vertex  $\Lambda^{eh}$ , however, may have unexpected implications. The electron-hole irreducible vertex is bound with the self-energy via the Ward identity. The singular behavior of the electron-hole irreducible vertex could then be transferred onto the self-energy. This can be made transparent by evaluating the function

$$\Delta W(\omega) = \frac{1}{N} \sum_{\mathbf{k}} [\Sigma(\mathbf{k}, E - \omega + i0^+) - \Sigma(\mathbf{k}, E + \omega + i0^+)] \quad (23)$$

in such a way that the self-energies are expressed in terms of the two-particle vertex  $\Lambda^{eh}$  according to the Fourier transform of Eq. (11). Doing so we finally find out<sup>7</sup> that, besides an analytic part, the function  $\Delta W$  contains also a singular term of the form

$$\Delta W_d^{sing}(\omega) \approx K \lambda n_F^2 \times \begin{cases} \frac{1}{\omega} \left| \frac{\omega}{Dk_F^2} \right|^{d/2} & \text{for } d \neq 4l, \\ \frac{1}{\omega} \left| \frac{\omega}{Dk_F^2} \right|^{d/2} \ln \left| \frac{Dk_F^2}{\omega} \right| & \text{for } d = 4l, \end{cases} \quad (24)$$

where  $K$  is a dimensionless constant,  $k_F$  stands for the Fermi momentum and  $d$  denotes spatial dimension. The non-analyticity of the self-energy, and therefore of the one-electron Green function, is unacceptable as it contradicts another very fundamental property — causality. Causality is a consequence of self-adjointness of the Hamiltonian, that is of reality of eigenenergies. It cannot be given up in any physically meaningful treatment. We are thus led to a surprising conclusion that the Ward identity (11) cannot survive to the thermodynamic limit of configurationally averaged Green functions. At least for real-energy differences denoted  $\omega$  in Eq. (23) and (24). This indicates that there must be a flaw in the seemingly straightforward extension of the Ward identity from finite to infinite configurationally averaged systems.

## V. APPROXIMATE ANALYTIC TREATMENTS

It is impossible to resolve rigorously the incompatibility of probability conservation and causality in infinite, configurationally averaged systems, since exact solutions are not provided. We hence have to resort to approximate treatments to trace down the problem and clues for a possible resolution.

It is natural to start with a mean-field solution for disordered electron systems, being the exact solution of the problem in infinite spatial dimensions. This limit amounts to the coherent-potential approximation. We have explicit expressions for all quantities in this approximation. The self-energy is determined from a Soven equation that can be cast into

$$G(z) = \left\langle [G^{-1}(z) + \Sigma(z) - V_i]^{-1} \right\rangle_{av} \quad (25a)$$

where  $G(z) = N^{-1} \sum_{\mathbf{k}} G(\mathbf{k}, z)$ . The two-particle irreducible vertex then is

$$\lambda(z_+, z_-) = \frac{1}{G(z_+)G(z_-)} \left[ 1 - \left\langle \frac{1}{1 + (\Sigma(z_+) - V_i) G(z_+)} \frac{1}{1 + (\Sigma(z_-) - V_i) G(z_-)} \right\rangle_{av} \right]^{-1} = \frac{\Sigma(z_+) - \Sigma(z_-)}{G(z_+) - G(z_-)}. \quad (25b)$$

The self-energy from the Soven equation (25a) can be proven analytic and the last equality in Eq. (25b) expresses the Ward identity. The conservation law is ful-

filled and apparently does not contradict causality.

The CPA is indeed a consistent theory, but only if we keep strictly to local quantities. To remain consis-

tent at the two-particle level we should hence consider only the local vertex being  $\gamma(z_+, z_-) = \lambda(z_+, z_-)/(1 - \lambda(z_+, z_-)G(z_+)G(z_-))$ . This local vertex, however, does not contain the diffusion pole. Velický derived in Ref. 8 the full two-particle vertex in the CPA in a form

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \frac{\lambda}{1 - \lambda\chi(\mathbf{q})} \quad (26)$$

where  $\chi$  is a two-electron bubble

$$\chi(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} G_+(\mathbf{k})G_-(\mathbf{k} + \mathbf{q}). \quad (27)$$

The CPA nonlocal two-particle vertex, Eq. (26), contains the diffusion pole precisely as in Eq. (19), see Ref. 6 for explicit calculation. Even at this level the CPA seems to be consistent. The CPA does not treat, however, the electron-hole and the electron-electron vertex equivalently. We have  $\Lambda^{eh} = \lambda$ , whereby there is no expression for the electron-electron irreducible vertex  $\Lambda^{ee}$ . The electron-hole symmetry for two-particle vertices is therefore broken in the mean-field solution. As a consequence of the violated electron-hole symmetry at the two-particle level we have no sign of localized states in the CPA.

To include localized states and to approach the Anderson metal-insulator transition we have to go beyond local approximations. Already the notion of weak localization needs a sum of infinite-many “crossed” two-particle diagrams (ladders from the electron-electron channel) leading to a singular electron-hole irreducible vertex. The importance of the electron-hole symmetry at the two-particle level and the diffusion pole in the electron-hole irreducible vertex was stressed and exploited by Vollhardt and Wölfle in their theory of Anderson localization.<sup>5</sup>

Theory of Vollhardt and Wölfle is a self-consistent approximation for the electron-hole and electron-electron irreducible vertices. Due to the complete electron-hole symmetry we obtain a nonlinear equation for a generic vertex. This vertex displays the diffusion pole of Eq. (19). Further on, the Ward identity (11) is assumed to hold. In this situation the two-particle irreducible vertex in the hydrodynamic limit ( $q \rightarrow 0$ ) contains only a single free adjustable parameter, the diffusion constant  $D$ . Anderson localization is signalled in this approach by vanishing of the diffusion constant  $D$ .

A diagrammatic expansion for two-particle irreducible functions is formally used to select an appropriate approximation in the Vollhardt-Wölfle theory. This theory, however, does not provide a similarly closed expression for the one-electron self-energy. Since the spectral behavior of the self-energy is not decisive for the existence of the Anderson localization transition, the self-energy in the one-electron propagators is taken from the weak-scattering limit, i. e. from the Born approximation. The Ward identity is used only to recover the diffusion pole, but not to determine the self-energy consistently so that it be compatible with the chosen approximate

vertex function. It is then evident that we cannot check compatibility of the Ward identity with causality within the Vollhardt-Wölfle theory. Due to Eq. (24) we cannot expect that a causal self-energy could be found to the approximate vertex resulting from the Vollhardt-Wölfle approach.

We can use another route to trace conservation laws in configurationally averaged infinite systems. Since the CPA obeys all restrictive conditions except for the two-particle electron-hole symmetry, we can try to correct this approximation just by implementing this missed feature. This can actually be achieved within the parquet approach providing a framework to sum systematically nonlocal vertex corrections to the CPA irreducible vertex.<sup>4</sup> We showed recently how to solve the parquet equations in electron-hole symmetric theories asymptotically exactly in the limit of high spatial dimensions.<sup>9</sup> The solution for the full two-particle vertex resembles that from the CPA, but the electron-hole symmetry is manifestly present. We obtain<sup>9</sup>

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \Lambda_0 \left[ \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \chi(\mathbf{q})} + \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{k} + \mathbf{k}' + \mathbf{q})}{1 - \bar{\Lambda}_0 \chi(\mathbf{k} + \mathbf{k}' + \mathbf{q})} \right] \quad (28)$$

where we used the local CPA vertex  $\gamma$  and denoted  $\Lambda_0 = \bar{\Lambda}_0/(1 + \bar{\Lambda}_0 G_+ G_-)$  and  $\bar{\chi}(\mathbf{q}) = \chi(\mathbf{q}) - G_+ G_-$ . The only local parameter to be determined from the parquet equation is  $\bar{\Lambda}_0$ . It fulfills an equation

$$\bar{\Lambda}_0 = \gamma + \bar{\Lambda}_0 \frac{1}{N} \sum_{\mathbf{q}} \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}. \quad (29)$$

It is clear that the CPA vertex, Eq. (26), is reproduced from Eq. (28) if we put  $\bar{\Lambda}_0 = \gamma$  in it and if the last term on its right-hand side is neglected. It is just the neglected term that restores the two-particle electron-hole symmetry. On the other hand, it is the same term that makes it difficult to comply with the Ward identity. The vertex  $\Gamma$  from Eq. (28) does not obey a Bethe-Salpeter equation. It is a sum of two solutions of the Bethe-Salpeter equations in the electron-hole and the electron-electron channels. It is hence unclear how to choose the self-energy so that it would fit the Ward identity.

To restore the diffusive behavior of the full vertex we have to use the Ward identity for a specific combination of energies and determine the self-energy from the irreducible vertex  $\Lambda_0$ . We use<sup>9</sup>

$$\Im \Sigma(E + i\eta) = \Lambda_0(E + i\eta, E - i\eta) \Im G(E + i\eta). \quad (30)$$

to resolve the imaginary part of the self-energy. The real part of the self-energy is then calculated from the Kramers-Kronig relation

$$\Re \Sigma(E + i\eta) = \Sigma_\infty + P \int_{-\infty}^{\infty} \frac{dE'}{\pi} \frac{\Im \Sigma(E' + i\eta)}{E' - E}. \quad (31)$$

In this way we construct a consistent approximation with the two-particle electron-hole symmetry and with

a causal self-energy that satisfies the Ward identity in a maximally possible way. Since the Ward identity was used in Eq. (30) only for imaginary energy difference in the vertex function, this solution is not in conflict with Eq. (24) where the energy difference is real.

The Ward identity does not hold in this solution for real energy differences. As a consequence the diffusion pole from Eq. (19) modifies to

$$\Phi_{EF}^{AR}(\mathbf{q}, \omega) \approx \frac{2\pi n_F}{-iA(\omega)\omega + D(\omega)q^2}. \quad (32)$$

The weight of the pole is no longer one,  $A(0) \geq 1$ . The quasistatic and hydrodynamic limit of the vertex function is then governed by two parameters, the diffusion constant  $D(0)$  and the weight of the diffusion pole (wave-function normalization)  $A(0)^{-1}$ . The Anderson localization transition is signalled here by vanishing of the weight of the diffusion pole  $A(0)^{-1} \rightarrow 0$  accompanied by vanishing of the effective diffusion constant  $D' = D(0)/A(0) \rightarrow 0$ .

## VI. PROBLEMS WITH A QUANTITATIVE DESCRIPTION OF LOCALIZED STATES IN TRANSLATIONALLY INVARIANT SYSTEMS

Our analysis disclosed a surprising fact that it is impossible to describe consistently disordered electron systems with averaged Green functions so that conservation of particle number would hold in the state space of Bloch waves, the eigenstates of the pure solids. Since the probability density is not conserved in the description with averaged functions, we have to ask where to can particles vanish?

To answer this question and to understand deviations from the Ward identity in averaged infinite systems, we recall that there are two very different types of states in the thermodynamic limit — extended and localized. The former are normalized to volume. Their normalization factor increases linearly with increasing volume. The latter are normalized to unity. Their normalization constant is effectively independent of the volume of large samples. This difference may seem to be a formal issue, but in fact it poses a principal obstacle for describing both types of states within one theoretical framework.

Each configuration of the random potential in a disordered system has its own representation space. It is the Hilbert space spanned over the eigenstates of the Hamiltonian with given values of the random potential. We can generally characterize the representation space via a decomposition of unity operator

$$\hat{1} = \frac{1}{N_{ext}} \sum_{\mathbf{x}}^{N_{ext}} |\mathbf{x}\rangle\langle\mathbf{x}| + \sum_{\nu}^{N_{loc}} |\nu\rangle\langle\nu| \quad (33)$$

where we distinguished extended eigenstates  $|\mathbf{x}\rangle$  and localized ones  $|\nu\rangle$ . The total number of eigenstates is

$N_{ext} + N_{loc} = N$ . To determine the eigenvalues of the configurationally dependent Hamiltonian we have to specify boundary conditions for the eigenvalue problem. We standardly use periodic boundary conditions for the extended states and asymptotic vanishing of the localized states. It is evident that we cannot describe localized states with periodic boundary conditions, unless they are periodically repeated as are e. g. Wannier states. Configurationally dependent localized states are confined to a specific finite part of the space and do not replicate themselves periodically, since one configuration is typically not translationally invariant.

We cannot effectively work with individual configurations, since we know neither the extended nor the localized eigenstates. Moreover, the ratio  $N_{loc}/N_{ext}$  varies from configuration to configuration. In the thermodynamic limit we are able to deal only with extended or periodically distributed localized states. We standardly use the Hilbert space spanned over the Bloch waves and assume that all relevant configurations of the random Hamiltonian can be accommodated in this space. There are no problems with delocalized eigenstates, since we have  $\langle\mathbf{x}|\mathbf{k}\rangle/\langle\mathbf{k}|\mathbf{k}\rangle = O(1)$ . However, the localized, translationally noninvariant states fall out from this Hilbert space, since  $\langle\nu|\mathbf{k}\rangle/\langle\mathbf{k}|\mathbf{k}\rangle = O(N^{-1})$ . Hence, if we have macroscopically many configurations with localized eigenstates, we observe deviations from the Ward identity for the averaged Green functions and probability will no longer be conserved in the space of asymptotically free states. Mathematically it means that the number of extended eigenstates  $N_{ext}$  is configurationally dependent and we cannot interchange the configurational averaging with the summation over the intermediate states in Eq. (9).

Evasion of localized states from the space of extended waves is a severe drawback of the description, since we loose the normalization of the density of states. To repair this we replace the missing localized states with extended ones so that we keep the number of available states always equal the number of the lattice sites  $N$ . Thereby we believe that the differences between the *exact unknown localized* and the *supplemented known Bloch waves* can be represented by corrections via the self-energy and other irreducible vertex functions. We recover the sum rule for the density of states, but the Ward identity at best only in the quasistatic limit  $\omega \rightarrow 0$ . This is the price we pay for our inability to describe the localized states in translationally invariant systems exactly.

## VII. CONCLUSIONS

We discussed in this paper applicability of conservation laws in disordered itinerant noninteracting systems. We showed that formal manipulations leading to conservation of the norm of the wave function are justifiable only for individual configurations of the random potential in finite volumes. Extensions of the conservation

laws via Ward identities to infinite systems demand a caution when dealing with infinite sums. In the thermodynamic limit we have to distinguish proper states from the Hilbert space with a finite norm (localized states) and generalized states with the norm (or the normalization constant) proportional to the volume (extended states). If we stay within individual configurations of the random potential we can well separate these two types of states and rely on the derivation of the Ward identities.

Problems arise, however, when we start to average over configurations to restore translational invariance. A generalization of the Ward identity to the averaged Green functions faces principal obstacles, when both types of states, localized and extended, are present. An extension of the Ward identity to the averaged functions can work when eigenstates of all relevant configurations are from the same Hilbert space. Based on the observed behavior of averaged systems we conclude that, whenever localized states become macroscopically relevant, we are

unable to find the proper Hilbert space to represent the localized eigenstates exactly. We have at our disposal practically only the Hilbert space spanned over the Bloch waves. The localized states are in the thermodynamic limit orthogonal to Bloch waves,  $\langle \nu | \mathbf{k} \rangle / \langle \mathbf{k} | \mathbf{k} \rangle = O(N^{-1})$ , and hence elusive to a quantitative description within the available Hilbert space. Since the space of Bloch waves is incomplete, probability is no longer conserved, when macroscopic portion of configurations contain localized states. Our standard assumption that configurational averaging does not influence the representation space and can be represented as averaging over rotations in the given Hilbert space is hence incorrect when quantum coherence between spatially distinct scattering events is taken into account.

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\* Electronic address: janiš@fzu.cz, kolorenc@fzu.cz

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